

**Optical Measurements and Modeling to Estimate Concentrations and
Fluxes of Organic Matter in the Southern Ocean**

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Abstract

This project was a collaboration between two Principal Investigators, Dr. Dariusz Stramski and Dr. Greg Mitchell of Scripps Institution of Oceanography, University of California San Diego. Our overall goal was to conduct optical measurements and modeling to estimate concentrations of organic matter in the Southern Ocean in support of the U.S. JGOFS Process Study in this region. Key variables and processes of high relevance to accomplish the JGOFS goals include time and space resolution of phytoplankton pigments, particulate organic carbon, and the formation and export of organic carbon. Our project focused on establishing the fundamental relationships for parameterization of these variables and processes in terms of the optical properties of seawater, and developing understanding of why the Southern Ocean differs from other low-latitude systems, or has differentiation within. Our approach builds upon historical observations that optical properties provide a useful proxy for key reservoirs of organic matter such as chlorophyll *a* (Chl) and particulate organic carbon (POC) concentrations, which are of relevance to the JGOFS objectives. We carried out detailed studies of *in situ* and water sample optical properties including spectral reflectance, absorption, beam attenuation, scattering, and backscattering coefficients. We evaluated the ability to estimate Chl from the spectral reflectance (ocean color) in the Southern Ocean. We examined relationships between the ocean optical properties and particulate organic carbon. We developed, for the first time, an algorithm for estimating particulate organic carbon concentration in the surface ocean from satellite imagery of ocean color (Stramski et al., 1999). With this algorithm, we obtained maps of POC distribution in the Southern Ocean showing the seasonal progression of POC in the austral spring-summer season. We also developed a semianalytical reflectance model for the investigated polar waters based on our field measurements of absorption and backscattering coefficients and Chl-dependent parameterizations of these coefficients (Reynolds et al., 2001). With this model, libraries of expected reflectance spectra for various chlorophyll concentrations can be generated with high spectral resolution for specific oceanic regions. In addition, our semianalytical reflectance model provided insight into the mechanisms which drive the empirical relationships between the ocean color and chlorophyll concentration. Our optical approach to the study of pigment and carbon concentrations will be directly relevant to development of system models and long-term monitoring of the Southern Ocean.

1. Objectives

The major objectives of our project were:

- (i) To examine bio-optical relationships in the Southern Ocean and explain why such relationships may differ from those at lower latitudes, or have differentiation within the Southern Ocean.
- (ii) To develop remote sensing algorithms for determining particulate organic carbon concentration and chlorophyll *a* concentration in the Southern Ocean.
- (iii) To provide optical data in support of the JGOFS goals.

2. Field campaigns

The initial phase of our JGOFS Southern Ocean project was administered by the NSF Office of Polar Programs (OPP 98-023836). During the first several months of the project before the field campaigns began, our effort concentrated on planning the cruise logistics, acquiring instruments, assembling the underwater instrumentation package for optical profiling, testing the instrumentation, and finally, shipping our cargo to Lyttleton in New Zealand (in September 1997). The new instruments, which were purchased for this project included the Hydrosicat-6 backscattering sensor (HobiLabs), temperature and conductivity sensors with a TC duct and a pump (SeaBird), two C-Star beam transmissometers (WetLabs) and a WETStar fluorometer for in situ chlorophyll detection (WetLabs). Our transmissometers were designed to measure the beam attenuation coefficient at 490 nm and 660 nm. The rest of the equipment of the profiling package was already available in Greg Mitchell's laboratory. This equipment included MER-2040 multichannel spectroradiometer (with a reference deck unit) for measuring spectral downwelling irradiance and upwelling radiance, two AC-9 instruments for in situ measurements of the spectral absorption and beam attenuation coefficients, a set of necessary pumps and a MODAPS data acquisition system. In addition to the in situ package, we shipped to New Zealand laboratory instruments (spectrophotometer, Coulter particle analyzer), computers, a van equipped with the filtration system designed as a wet lab, and a great variety of materials and supplies.

We participated in three cruises in the Antarctic, working for over 100 days at sea from November 5, 1997 through March 19, 1998, a period of 3.5 months. The first cruise was the Process IV in the Ross Sea on the Nathaniel B. Palmer with Dr. W. Smith as a Chief Scientist (40 days). The two other cruises were on R/V Roger Revelle in the Antarctic Polar Front Zone (APFZ); the Survey II led by Dr. K. Coale (30 days) and the Process II led by Dr. W. Gardner (34 days). Three people from our team participated in the Ross Sea cruise (Mitchell, Stramski, and Reynolds) and two people in each APFZ cruise (Wieland/Bichnevicius and Reynolds/Wieland). Overall we committed more than 240 person-days to our field program. This represents a very intensive field effort that resulted in the collection of extensive and unique optical data set.

During the Ross Sea Process IV cruise we completed over 50 in situ casts with our optical profiling system, each down to a depth of 200 m. These measurements allowed us to collect simultaneously the information on the spectral characteristics of the downwelling and upwelling light fields and inherent optical properties (IOPs). One of the most unique features of our system was the capability to measure the spectral backscattering coefficient at six wavelengths. Each in situ optical cast was accompanied by CTD cast which provided us with water samples from several discrete depths (typically 4 to 8 depths from the top 200 m layer) for a variety of laboratory analyses. These analyses included the measurements of absorption spectra of particulate and soluble materials with a Cary 1 bench-top double beam spectrophotometer. The

particulate spectra were partitioned into phytoplankton and detrital components using the method based on methanol treatment. In addition to these routine absorption measurements, we carried out specialized absorption experiments using another spectrophotometer equipped with 15-cm integrating sphere (Perkin Elmer Lambda 18). These experiments aimed at determining the pathlength amplification factor for the filter-pad technique and tests of filter-transfer-freeze technique. In these experiments, measurements were done on filters and suspensions. The suspensions were prepared by filtering large volumes of seawater and subsequent concentration of the collected particles by resuspension in smaller volumes of seawater. Overall our data from routine and specialized spectrophotometric measurements include over 1,000 spectral scans, each scan covering the spectral region from UV to near infrared with 1 nm resolution. In addition, we used Coulter particle analyzer to measure the concentration and size distribution of particles larger than about 2 μm in diameter. We also collected samples for pigments and particulate organic carbon (POC) for post-cruise analysis in laboratory. In regard to the APFZ cruises, we carried out the same measurements and analyses as in the Ross Sea with the exception of spectrophotometric experiments on pathlength amplification and filter-transfer-freeze method.

Most significant variables, which were directly measured or derived from the measurements include the spectral downwelling irradiance and upwelling radiance, the spectral reflectance, the spectral beam attenuation coefficient, absorption coefficient (partitioned into contributions by phytoplankton, detrital particles and dissolved matter), scattering and backscattering coefficients, particle size distribution, and pigment and particulate organic carbon (POC) concentrations in sea water.

3. Data processing and management

Upon completion of the field work in the Southern Ocean, all in situ optical instruments were returned to their respective manufacturers for re-calibration. Results of these calibrations were compared with pre-cruise values and, when available, long term calibration trends, and appropriate conversion factors for processing raw data to engineering units were derived. In addition to standard calibrations, additional experiments to examine measurement sensitivity to low temperatures were performed for some instruments (e.g. Wet Labs C-Star beam transmissometer).

Following calibration determinations, we completed the processing of bio-optical profiles collected with the in situ instrument package. Processing of downwelling irradiance, $E_d(\lambda)$, and upwelling radiance, $L_u(\lambda)$, collected from the MER-2040 spectroradiometer was done with a modified version of the BBOP data processing system. In order to ensure compatible depth values with the JGOFS CTD-Rosette system, a calibration of the MER depth sensor was performed using linear regression analysis comparing depths of a large number of distinct features (e.g. transmission minimum, fluorescence maximum, bottom of the mixed layer) in profiles measured with both systems. All raw data profiles were broken into separate downcast and upcast files, visually inspected for sources of error and contamination (e.g. influence of ship shadowing or wave focusing), and given a quality ranking. Based upon this visual inspection, depth intervals for vertical binning and extrapolation to surface values were chosen and used to create ASCII files containing calibrated data. A similar approach was employed for processing of data collected by ancillary sensors controlled by the MER, including stimulated chlorophyll fluorescence, beam attenuation, conductivity, and temperature.

The Hydrosat-6 spectral backscattering sensor is a new commercial instrument, and we devoted a significant effort to critically examine the quality of this measurement and to develop an appropriate processing scheme. Computer programs (MatLab 5.1) were written for standard processing of raw backscattering profiles (e.g. vertical binning, de-spiking) and conversion to

physical units. A unique feature of our processing scheme was the inclusion of measured values of the spectral beam attenuation coefficient for calculation of the necessary attenuation correction factor. This correction was particularly significant in highly turbid waters encountered at Ross Sea stations located within blooms of the Prymnesiophyte *Phaeocystis antarctica*.

Spectral absorption coefficients of particulate and soluble material, measured aboard ship with a Varian Cary spectrophotometer, were processed and converted to physical units. Based upon our at-sea experiments examining the pathlength amplification ("beta") factor of natural particle assemblages, the Mitchell 1992 equation was chosen as the default processing algorithm. Because of the relatively low amounts of colored dissolved material in these waters (and hence low measurement signal), processing of soluble absorption measurements required a thorough analysis of instrument sensitivity and baselines. To minimize the influence of instrument noise, soluble absorption data were fit to an exponential spectral dependence law. The size distribution of particle assemblages, measured with a Coulter Counter, were processed to yield absolute particle numbers per unit volume.

Samples returned to the laboratory for determining particulate organic carbon (POC) and HPLC pigment determinations were analyzed.

To facilitate data analyses and linking with the US JGOFS database, we are in the process of generating a relational database of our biological and optical measurements in the Southern Ocean (Microsoft Access). In this database in situ optical profiles can be easily linked to analyses of discrete water samples (e.g. particulate absorption spectra, particle size distribution) and hydrographic data provided by the JGOFS database.

4. Data analysis and modeling

To accomplish the objectives of our project, we carried out advanced data analyses and modeling studies. Below we summarize the most important results.

4.1 *SeaWiFS validation*

We performed a validation exercise comparing SeaWiFS-retrieved normalized water-leaving radiances (L_{WN}) with in situ data collected concurrently (± 4 hours). HRPT data received at McMurdo Station, Antarctica, were processed to yield L_{WN} using SeaDAS 3.2 software, with satellite values derived as averages over 3×3 pixel areas centered at the in situ measurement. Because of persistent cloud cover and large mesoscale variability in surface Chl concentrations, only 3 rigorous matchups were possible in the Ross Sea region (all on Dec-1-1997). Although limited in number, these comparisons reveal significant under-estimation of the SeaWiFS-retrieved L_{WN} compared to in situ measurements. The differences are generally smallest in the 555 nm band, and largest at shorter wavelengths; the magnitude of under-estimation in the shorter wavelength bands appears to increase at high Chl concentration. These findings are consistent with validation data reported by other NASA investigators in diverse oceanic regions. These results, combined with our similar data from the California Current Region, were presented at the Fall 1998 AGU Meeting in San Francisco (Kahru and Mitchell 1998), and at the Southern Ocean JGOFS AESOPS Workshop in Knoxville (Mitchell et al., 1998).

4.2 *Empirical Chl algorithm*

The Ocean Color 2 (OC2) chlorophyll algorithm is presently used by NASA in the operational processing of SeaWiFS data. This empirical algorithm uses the ratio of remote sensing reflectances (R_{rs}) at 490 and 555 nm to estimate chlorophyll *a* concentration, with the

coefficients derived by a statistical fit to a data set of bio-optical measurements comprising the SeaBAM data set (it is worth noting that no Antarctic measurements are included in this SeaBAM data set). More recently, NASA announced a revised version of the OC2 (OC2-v2), which was intended to reduce the drastic over-estimation of Chl in high biomass waters produced by the original algorithm.

We have compared the performance of the OC2-v2 algorithm with our in situ optical measurements from the Southern Ocean. No strong regional differentiation in the Chl vs $R_{rs}(490)/R_{rs}(555)$ relationship between the Ross Sea and Antarctic Polar Front regions was observed. Our data suggest that for low to moderate surface Chl concentrations (~ 0.1 - 2 mg m^{-3}), the OC2-v2 algorithm leads to consistent under-prediction of Chl concentration by nearly 50%. For stations with high surface Chl (e.g. bloom stations), the opposite situation is observed and Chl concentration is severely over-estimated ($>300\%$). These findings are consistent with previous observations that bio-optical relationships in the Southern Ocean often differ significantly from lower-latitude regions, and underscore the need for development of specific regional empirical algorithms to obtain more accurate estimates of Chl and primary production from ocean color remote sensing. These results were presented at the Fall 1998 AGU meeting (Reynolds et al. 1998) and the preparation of a manuscript on this subject is in progress.

4.3. POC-optics relationships and POC satellite algorithm

The development of optical tools to study the time-varying, large scale distribution of particulate organic carbon (POC) in the Southern Ocean was a major focus of our project. Using data collected during the Ross Sea cruise, we have demonstrated strong correlations between the concentration of POC and two inherent optical properties of seawater, the spectral beam attenuation and backscattering coefficients for particles. The empirical relationship obtained between POC and beam attenuation in the Ross Sea is remarkably similar to results obtained from other oceanic regions. This finding has important implications for the large scale determination of POC, as beam transmission is one of the few inherent optical properties of seawater which can be routinely monitored from sensors mounted on ships, towed vehicles, and moorings. These results were presented at the November 1998 Ocean Optics XIV Conference in Kailua-Kona, Hawaii (Stramski et al. 1998).

The strong correlation observed between POC and backscattering is also an exciting result of our work as backscattering can, in principle, be derived from ocean reflectance. Our study provided evidence, for the first time, that measurement of the spectral backscattering coefficient may provide a means to estimate POC from satellite ocean color imagery. Following this line of reasoning, we used our data set from both the Ross Sea and Polar Front region to develop a novel empirical model for deriving maps of near-surface POC from satellite data. We applied this algorithm to SeaWiFS data to produce time series of monthly images of POC in the Southern Ocean around Antarctica. This time series clearly illustrates the seasonal progression of the distribution of POC in the Southern Ocean for the 1997-98 austral spring-summer season. The results show the presence of a distinct zonal band of elevated POC concentrations in the month of December, coinciding with the Polar Front Zone surrounding Antarctica. In addition, numerous and at times widespread areas of POC in December and January are observed, which are consistent with phytoplankton blooms as seen by satellite-derived images of Chl concentration. Our calculations suggest that the net seasonal change in the surface POC pool of the Southern Ocean (the upper 100-m layer of the ocean) between the summer maximum (December-January) and winter minimum (June-July) is > 0.3 gigatons of carbon. We believe that this work will lead to significant advances in understanding of the role of the oceans in global carbon cycle. A paper describing these results was published in *Science* (Stramski et al. 1999),

and two presentations related to this subject were given at the 2000 Ocean Sciences Meeting in San Antonio (Stramski et al., 1999; Mitchell et al., 1999).

4.4. Semianalytical reflectance model

A semianalytical model was developed for the prediction of spectral remote-sensing reflectance (R_{rs}) as a function of chlorophyll *a* concentration (Chl) for two regions within the Southern Ocean; the Ross Sea and the Antarctic Polar Front Zone (APFZ). The model is based upon Chl-dependent parameterizations of the spectral absorption, $a(\lambda)$, and backscattering, $bb(\lambda)$, coefficients of seawater which were derived from field measurements. The relationships between $a(\lambda)$ and Chl were similar in both regions, but for comparable Chl the particulate backscattering was on average four times greater in the APFZ. Measurements of particle size distributions suggest that particle assemblages in the APFZ were characterized by a greater predominance of smaller particles, consistent with the observed regional differences in backscattering properties. The model was used to examine the separate influences of absorption and backscattering on the blue to green ratio of reflectance, $R_{rs}(490)/R_{rs}(555)$. Variability in the spectral absorption ratio, resulting principally from changes in the relative contribution of water to total absorption in each band, contributes >75% to changes in the $R_{rs}(490)/R_{rs}(555)$ ratio as a function of Chl. However, variability in the spectral backscattering ratio appears to be the primary cause for the observed differentiation in the R_{rs} versus Chl relationships between the two regions. With this model, libraries of expected reflectance spectra for various chlorophyll concentrations can be generated with high spectral resolution for specific oceanic regions. In addition, our semianalytical reflectance model provided insight into the mechanisms which drive the empirical relationships between the ocean color and chlorophyll concentration. A paper describing these results was published in *Journal of Geophysical Research* (Reynolds et al., 2001) and this model was also presented at the ASLO 2001 Aquatic Sciences Meeting in Albuquerque (Reynolds et al., 2001).

5. Publications and conference/workshop presentations

We published two major research articles and we made eight conference/workshop presentations. Below is a list of these contributions in chronological order.

Research articles:

Stramski, D., R.A. Reynolds, M. Kahru, and B.G. Mitchell. 1999. Estimation of particulate organic carbon in the ocean from satellite remote sensing. *Science*, 285: 239-242.

Reynolds, R. A., D. Stramski, and B. G. Mitchell. 2001. A chlorophyll-dependent semianalytical reflectance model derived from field measurements of absorption and backscattering coefficients within the Southern Ocean. *J. Geophys. Res.* 106 (C4): 7125-7138.

Conference/Workshop presentations:

Mitchell, B.G., M. Kahru, C. Xi, and R.A. Reynolds. 1998. SeaWiFS data in the Ross Sea on December 1, 1997: A preliminary validation study. US Southern Ocean JGOFS AESOPS Workshop, June 17-24, 1998. Knoxville, Tn.

- Mitchell, B.G., D. Stramski, and R.A. Reynolds. 1998. Optical measurements and modeling to estimate concentrations and fluxes of organic matter within the Southern Ocean. US Southern Ocean JGOFS AESOPS workshop, June 17-24, 1998. Knoxville, Tn.
- Stramski, D., R.A. Reynolds, and B.G. Mitchell. 1998. Relationships between the backscattering coefficient, beam attenuation coefficient, and particulate matter concentrations in the Ross Sea. Conference proceedings of Ocean Optics XIV, November 10-13, 1998. Kailua-Kona, HI.
- Kahru, M. and B.G. Mitchell. 1998. Empirical chlorophyll algorithm for the California Current. EOS, Transactions, American Geophysical Union. 79(45): F430.
- Reynolds, R.A., M. Kahru, J.D. Wieland, D. Stramski, and B.G. Mitchell. 1998. An evaluation of SeaWiFS ocean color chlorophyll algorithms within the Southern Ocean. EOS, Transactions, American Geophysical Union. 79(45): F430.
- Mitchell, B. G., M. Kahru, R. A. Reynolds, J. D. Wieland, and D. Stramski. 1999. Satellite estimation of seasonal variations in organic carbon to chlorophyll-a ratios in the Southern Ocean and interpretation of carbon flux dynamics. Supplement to EOS, Transactions, American Geophysical Union, 80(49): OS27.
- Stramski, D., R. Reynolds, M. Kahru, J. Wieland, and G. Mitchell. 1999. Geographic distribution and seasonal variations in particulate organic carbon within the Southern Ocean as determined from satellite imagery of ocean color. Supplement to EOS, Transactions, American Geophysical Union, 80(49): OS27.
- Reynolds, R. A., D. Stramski, and B. G. Mitchell. 2001. A semianalytical reflectance model derived from field measurements of absorption and backscattering coefficients within the Southern Ocean. ASLO 2001 Aquatic Sciences Meeting, Albuquerque, New Mexico. Abstract Book, p.118.

6. Personnel

Dr. Dariusz Stramski from Marine Physical Laboratory, Scripps Institution of Oceanography, and Dr. B. Greg Mitchell from Marine Research Division, Scripps Institution of Oceanography, were Principal Investigators of this project. Dr. Mati Kahru, Associate Investigator in Mitchell's lab, and Dr. Rick Reynolds, Postgraduate Researcher in Mitchell's and Stramski's lab, were involved and supported by this project. The technical staff in Mitchell's lab, J. Wieland and B. Bichnevicius were also involved and supported by the project.